Occidental Chemical Corporation ***OxyChem.***
A subsidiary of Occidental Petroleum Corporation

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Via Federal Express

February 16, 2007

Charles M. Auer
Director, Office of Pollution Prevention and Toxics (OPPT) (7401M)
Environmental Protection Agency
1200 Pennsylvania Ave., NW
Washington, DC 20460-001

RE: TSCA Section 8(d) Health and Safety Data Reporting Rule - Submission EPA-HQ-OPPT-2005-0055

Dear Mr. Auer:

Occidental Chemical Corporation (OxyChem) is in receipt of your November 13, 2006 letter which granted a 90-day extension for submittal of data in response to the TSCA Section 8(d) Health and Safety Data Reporting rule issued by EPA on August 16, 2006. The extension was from November 28, 2006 to February 26, 2007.

In response to the 8(d) rule, OxyChem is submitting robust summaries for the following materials:

CAS#: 98-56-6 Chemical: Benzene, 1-chloro-4-(trifluoromethyl)-
CAS#: 5216-25-1 Chemical: Benzene, 1-chloro-4-(trichloromethyl)-
CAS#: 25168-05-2 Chemical: Benzene, Chloromethyl-

OxyChem has determined that it has no unpublished studies that meet the data quality requirements for submission for CAS# 2905-62-6 (Benzoyl chloride, 3,5-dichloro-).

If you need additional information, please contact Debbie Schober at (972) 404-4969.

Sincerely,

CONTAINS NO CBI

Attachments

8607000004 7

302855

IUCLID Data Set

CAS# 98-56-6

Occidental Chemical Corporation

1.0 General Information

1.0.1 Substance Information

A. **CAS No.:** 98-56-6

B. **Chemical:** 1-Chloro-4-(trifluoromethyl)benzene

C. **Generic Name:**

D. **EINECS Name:**

E. **Molecular Formula:** $C_7H_4ClF_3$

F. **Molecular Weight:** 180.6

1.02 OECD Information

Company: Occidental Chemical Corporation
Creation date:

Company: Brock Scientific Consulting, LLC on behalf of Occidental Chemical Corp.

Printing Date:
Date of Last Update:

Number of Pages: 13

Chapter (profile): 1, 2, 5
Reliability (profile): without reliability, 1

1.03 Details of Chemical Category

1.1 General Substance Information

A. **Type of Substance:** Organic

B. **Physical State:** Liquid

C. **Purity:** 96-98%

D. **Color:** Water-white

E. **Odor:** Aromatic

1.2 Impurities

- 1-Chloro-2-(trifluoromethyl)benzene (CAS# 88-16-4)
- High boilers (No CAS#)
- 1,2-Dichloro-4-(trifluoromethyl)benzene (CAS# 328-84-7)

- 2,4-Dichloro-1-(trifluoromethyl)benzene (CAS# 320-60-5)

1.3 Additives

1.4 Synonyms

- p-(Chloropheny)-trifluoromethane
- 1-(Trifluoromethyl)-4-chlorobenzene
- PCBTF
- p-ClBTF
- 4-Chloro-alpha, alpha, alpha, alpha-trifluorotoluene

1.5 Quantity

1.6 Use Patterns

1.7 Sources of Exposure

1.8 Additional Information

In Sections 5.2 and 5.3, the test article is stated to be "PCBTF/TCMB Crude". TCMB is trichloromethoxybenzene. PCBTF was used as the feedstock for the manufacture of TCMB. The test article, however, did not contain TCMB.

2.0 Physical-Chemical Data

2.1 Melting Point

2.2 Boiling Point

2.3 Density

2.4 Vapor Pressure

2.5 Partition Coefficient

2.6.1 Water Solubility

Value: 60 mg/L
Qualitative: Visualization
Method: PCBTF (0.2015 g) was dissolved quantitatively in acetone to a concentration of 100 µg/µL. Volumes of the acetone-PCBTF solutions were injected into separate 8.8 mL screw cap vials that were fitted with a Teflon septum that contained water. The volumes injected were 1, 2, 3, 5, 6, 7 and 10 µL. The vials were vigorously shaken and then observed for solution clarity against a lighted background. After 5 minutes, the vials were again shaken and observed for a cloudy appearance of the PCBTF colloid suspension.

Year: 1983
GLP: No
Result: The solubility estimate assumed that the injection of the acetone "spiking" solution into the water would produce a colloidal suspension which would solubilize in about 5 min if the amount of PCBTF was less than the matrix solubility limit. The solubility also was limited by the ability to visually detect a colloid suspension.
Source: Dietz, 1983.
Reliability: 4 – Not Assignable

2.6.2.1.1 Other Solvents

Value: 60 mg/L
Qualitative: Visualization
Method: PCBTF (0.2015 g) was dissolved quantitatively in acetone to a concentration of 100 µg/µL. Volumes of the acetone-PCBTF solutions were injected into separate 8.8 mL screw cap vials that were fitted with a Teflon septum that contained diluted HCl. The concentration of HCl is assumed to be 10% based on data for another chemical used in these studies, but this is not specifically stated. The volumes injected were 1, 2, 3, 5, 6, 7 and 10 µL. The vials were vigorously shaken and then observed for solution clarity against a lighted background. After 5 minutes, the vials were again shaken and observed for a cloudy appearance of the PCBTF colloid suspension.
Year: 1983
GLP: No
Result: The solubility estimate assumed that the injection of the acetone "spiking" solution into the diluted HCl would produce a colloidal suspension which would solubilize in about 5 min if the amount of PCBTF was less than the matrix solubility limit. The solubility also was limited by the ability to visually detect a colloid suspension.
Source: Dietz, 1983.
Reliability: 4 – Not Assignable

Value: 10 mg/L
Qualitative: Visualization
Method: PCBTF (0.2015 g) was dissolved quantitatively in acetone to a concentration of 100 µg/µL. Volumes of the acetone-PCBTF solutions were injected into separate 8.8 mL screw cap vials that were fitted with a Teflon septum that contained a brine solution (unknown salt concentration). The volumes injected were 1, 2, 3, 5, 6, 7 and 10 µL. The vials were vigorously shaken and then observed for solution clarity against a lighted background. After 5 minutes, the vials were again shaken and observed for a cloudy appearance of the PCBTF colloid suspension.
Year: 1983
GLP: No
Result: The solubility estimate assumed that the injection of the acetone "spiking" solution into the brine solution would produce a colloidal suspension which would solubilize in about 5 min if the amount of PCBTF was less than the matrix solubility limit. The solubility also was limited by the ability to visually detect a colloid suspension.

Source: Dietz, 1983.
Reliability: 4 – Not Assignable

2.6.2 Surface Tension

2.7 Flash Point

2.8 Auto Flammability

2.9 Flammability

2.10 Explosive Properties

2.11 Oxidizing Properties

2.12 Oxidation/Reduction Potential

2.13 Additional Remarks

3.0 Environmental Fate and Pathways

3.1 Stability

A. Photodegradation

B. Stability in Water

C. Stability in Soil

3.2 Monitoring Data (Environment)

3.3 Transport and Distribution

3.3.1 Transport between Environmental Compartments

3.3.2 Distribution

3.4 Aerobic Degradation

3.5 BOD5, COD or BOD5/COD Ratio

3.6 *Bioaccumulation*

3.7 Additional Remarks

4.0 Environmental Toxicity

4.1 Acute Toxicity to Fish

4.2 Acute Toxicity to Aquatic Invertebrates

4.3 Toxicity to Aquatic Plants

4.4 Toxicity to Microorganisms

4.5 Chronic Toxicity to Aquatic Organisms

A. Chronic Toxicity to Fish

B. Chronic Toxicity to Aquatic Invertebrates

4.6 Terrestrial Organisms

A. Toxicity to Soil Dwelling Organisms

B. Toxicity to Terrestrial Plants

C. Toxicity to other Non-Mammalian Terrestrial Species

4.6.1 Toxicity to Sediment Dwelling Organisms

4.7 Biological Effects Monitoring

4.8 Biotransformation and Kinetics

4.9 Additional Remarks

5.0 Mammalian Toxicity

5.1 Toxicokinetics, Metabolism and Distribution

5.2 Acute Toxicity

A. Acute Oral Toxicity

Type: LD50
Species: Rat

Strain: Sprague Dawley
Sex: Male/Female
Number of Animals: 5/sex
Vehicle: None
Value: >1250 mg/kg
Method: Single oral dose administered to fasted rats. Animals observed daily for 14 days for clinical signs of toxicity and mortality. Body weights were recorded on days 1, 7 and 14 with gross necropsy of the thoracic and abdominal cavities conducted at day 14.
Year: 2000
GLP: Yes
Test substance: PCBTF/TCMB Crude
Result: No mortalities occurred and no clinical signs of toxicity were noted. All animals gained weight during the 14-day observation time. No gross abnormalities were observed.
Source: Product Safety Labs, 2000.
Reliability: 1- Reliable without restrictions

B. Acute Inhalation Toxicity

Type: LC50
Species: Rat
Strain: Sprague Dawley
Sex: Male/Female
Number of Animals: 5/sex
Vehicle: None
Duration: 4 hr
Value: >0.029 mg/L
Method: Single inhalation exposure at a nominal concentration of 1 mg/L. Animals observed daily for 14 days for clinical signs of toxicity and mortality. Body weights were recorded on days 1, 7 and 14 with gross necropsy of the thoracic and abdominal cavities conducted at day 14. Particle size distribution measured during exposure.
Year: 2000
GLP: Yes
Test substance: PCBTF/TCMB Crude
Result: No mortalities occurred. Clinical signs of toxicity were noted in all exposed rats and consisted of hypoactivity, irregular respiration, hunched posture and ocular discharge following exposure. No clinical signs were noted in any of the animals by day 3 following exposure. All animals gained weight during the 14-day observation time. No gross abnormalities were observed. The gravimetric chamber concentration was 0.029 mg/L.
Source: Product Safety Labs, 2000.
Reliability: 1- Reliable without restrictions

C. Acute Dermal Toxicity

Type: LD50
Species: Rat

Strain: Sprague Dawley
Sex: Male/Female
Number of Animals: 5/sex
Vehicle: None
Duration: 24 hr
Value: >2000 mg/kg
Method: Single topical dose applied to the clipped, intact skin of rats under an occlusive patch for 24 hr. Animals observed daily for 14 days for clinical signs of toxicity and mortality. Body weights were recorded on days 1, 7 and 14 with gross necropsy of the thoracic and abdominal cavities conducted at day 14.
Year: 2000
GLP: Yes
Test substance: PCBTF/TCMB Crude
Result: No mortalities occurred and no clinical signs of toxicity were noted. Erythema and edema were noted in the application site of all treated rats but the irritation had resolved in all animals by day 7. All animals gained weight during the 14-day observation time. No gross abnormalities were observed.
Source: Product Safety Labs, 2000.
Reliability: 1- Reliable without restrictions

D. Acute Toxicity, Other Routes

5.3 Corrosiveness and Irritation

A. Skin Irritation

Species: Rabbit
Strain: New Zealand White
Concentration: 100%
Dose: 0.5 mL
Exposure Time: 3 min, 1 and 4 hr
Number of Animals: 3 male rabbits
Classification: Irritant
Method: The test substance applied to three different test sites of the intact skin of rabbits. The sites were covered with a gauze pad, but the sites were not occluded. The patch was removed after the appropriate time and any residual substance removed with water. All sites were evaluated for irritation/corrosion at 1 hr following patch removal. Subsequent evaluations conducted at 24, 48, 72 hr and at 7, 10 and 14 days following patch removal. Irritation scored by the method of Draize.
Year: 2000
GLP: Yes
Test substance: PCBTF/TCMB Crude
Result: Very slight to well-defined erythema and very slight to slight edema observed in all test sites through day 10. By day 14, all irritation had resolved although desquamation was evident in all treated sites from day 7 through day 14.

3-Minute Exposure

Animal Number	Time after Patch Removal	Time after 4-hr Patch Removal					
	1 hr	24 hr	48 hr	72 hr	7 Days	10 Days	14 Days
1063	1/0	1/1*	1/1	0/0	0/0	0/0	0/0
1064	1/0	1/1	1/1	1/1	1/1	1/1	0/0
1065	1/1	1/1	1/1	1/1	1/1	1/1	0/0

* Draize scores presented as erythema/edema

1-Hour Exposure

Animal Number	Time after Patch Removal	Time after 4-hr Patch Removal					
	1 hr	24 hr	48 hr	72 hr	7 Days	10 Days	14 Days
1063	1/1	1/2*	1/2	1/1	0/01/1	0/0	0/0
1064	1/1	1/2	1/2	1/2	1/1	1/1	0/0
1065	1/1	1/2	1/2	1/2	1/1	1/1	0/0

* Draize scores presented as erythema/edema

4-Hour Exposure

Animal Number	Time after Patch Removal	Time after 4-hr Patch Removal					
	1 hr	24 hr	48 hr	72 hr	7 Days	10 Days	14 Days
1063	1/1	2/1*	2/1	2/1	1/1	1/1	0/0
1064	1/1	1/2	1/2	2/2	1/1	1/1	0/0
1065	1/0	1/2	1/2	1/2	1/1	1/1	0/0

* Draize scores presented as erythema/edema

Source: Product Safety Labs, 2000.
Reliability: 1- Reliable without restrictions

B. Eye Irritation

Species: Rabbit
Strain: New Zealand White
Concentration: 100%
Dose: 0.1 mL
Exposure Time: After instillation, the eyes were held closed for about 1 sec.
Number of Animals: 2 male and 1 female rabbit
Classification: Irritant
Method: The test substance was instilled into the conjunctival sac of the right eye; the left eye served as the control. Ocular irritation was evaluated at 1, 24, 48, 72 hr and at 4 and 7 days following instillation. Irritation scored by the method of Draize.
Year: 2000
GLP: Yes
Test substance: PCBTF/TCMB Crude
Result: No corneal opacity was observed during the study. At 1 hr, conjunctivitis was noted in all treated eyes. By day 7, all irritation had resolved.

Rabbit Number	Scoring Time (hr)	Corneal Opacity	Iritis	Conjunctiva		
				Redness	Chemosis	Discharge
1078	1	0	0	2	1	2
	24	0	0	2	1	1
	48	0	0	2	1	1
	72	0	0	1	1	1
	4 days	0	0	1	1	1
	7 days	0	0	0	0	0
1079	1	0	0	1	1	1
	24	0	0	1	1	1
	48	0	0	0	0	1
	72	0	0	0	0	1
	4 days	0	0	0	0	1
	7 days	0	0	0	0	0
1080	1	0	0	2	1	2
	24	0	0	1	1	1
	48	0	0	0	0	1
	72	0	0	0	1	1
	4 days	0	0	0	0	1
	7 days	0	0	0	0	0

Source: Product Safety Labs, 2000.
Reliability: 1- Reliable without restrictions

5.4 Sensitization

5.5 Repeated Dose Toxicity

Species: Rats
Strain: Sprague-Dawley
Sex: Male and female
Route of administration: Gavage
Exposure period: 14 Days
Frequency of treatment: Daily
Observation period: 14 Days
Doses: 7.5, 15, 30, 60, 120 mg/kg
Control Group: Corn oil
NOAEL: 120 mg/kg
Method: Rats (3/sex/group) were treated daily by gavage at a dose volume of 4 mL/kg. The animals were observed twice daily for clinical signs of toxicity and moribundity and mortality. Body weights were recorded twice weekly, and food consumption was determined weekly. At termination, blood was collected from one animal/sex/group for clinical pathology. The animals were subjected to a gross necropsy, and the spleen, liver and kidneys weighed.
Year: 1980
GLP: Yes

Test substance: As described in Section 1.1
Result: No compound-related effects were observed on clinical signs of toxicity, body weight or food consumption. No effects were observed on clinical pathology measures or organ weights. No gross pathology findings were observed.
Source: Elars Bioresearch Laboratories, 1980.
Reliability: 2- Reliable with restrictions

Species: Rats
Strain: Sprague-Dawley
Sex: Male and female
Route of administration: Gavage
Exposure period: 14 Days
Frequency of treatment: Daily
Observation period: 14 Days
Doses: 7.5, 15, 30, 60, 120 mg/kg
Control Group: Corn oil
NOAEL: 60 mg/kg
Method: Rats (5/sex/group) were treated daily by gavage at a dose volume of 2 mL for males and 1 mL for females. The animals were observed twice daily for clinical signs of toxicity and moribundity and mortality. Body weights were recorded daily with food consumption measured weekly. At termination, blood was collected from each animal for hematology measurement. The animals were subjected to a gross necropsy, and the liver weighed.
Year: 1979
GLP: No
Test substance: As described in Section 1.1
Result: One high-dose male was sacrificed prior to necropsy. All other animals survived the study duration. Body weights and food consumption were comparable across all groups. No effects were observed on hematology measures or liver weights. Liver and kidney lesions were seen in males and females with a greater incidence among male rats. Histologically, congestion of the kidneys was noted in males at most dose levels with hemorrhage noted at 60 and 120 mg/kg. These findings were not considered to be of toxicological significance. Hylaine droplet formation in the kidney was noted in 3/5 males in the high dose group and was considered compound-related. No significant findings were noted in females.
Source: Raltech Scientific Services, 1979.
Reliability: 2- Reliable with restrictions

Species: Rats
Strain: Sprague-Dawley
Sex: Male and female
Route of administration: Diet
Exposure period: 28 Days
Frequency of treatment: Daily
Observation period: 28 Days

Doses: 2, 20, 200, 2000 ppm in diet
Control Group: Corn oil added to control diet
NOAEL: 2000 ppm
Method: Rats (5/sex/group) were provided treated diet daily. The animals were observed twice daily for clinical signs of toxicity and moribundity and mortality. Body weights were and food consumption were recorded weekly. At termination, plasma and urine were collected from each animal for determining concentrations of PCBTF. The animals were subjected to a gross necropsy.
Year: 1978
GLP: No
Test substance: As described in Section 1.1. Subsequent analysis showed up to 15% of unidentified impurities.
Result: No compound-related effects were observed on clinical signs of toxicity, body weight or food consumption. No gross pathology findings were observed. PCBTF was not detected in either the plasma or urine of the treated rats at any concentration (limit of detection 0.5 ppm).
Source: Raltech Scientific Services, 1978.
Reliability: 2- Reliable with restrictions

5.6 Genetic Toxicity 'in Vitro'

A. Gene Mutation

B. Chromosomal Aberration

5.7 Genetic Toxicity 'in Vivo'

5.8 Carcinogenicity

5.9 Toxicity to Reproduction

A. Fertility

B. Developmental Toxicity/Teratogenicity

5.10 Other Relevant Information

A. Neurotoxicity

B. Other

5.11 Experience with Human Exposure

6.0 References:

Dietz, E.A. 1983. Memo to V. Rande: Solubility of p-chlorobenzotriflouride and p-chlorobenzoic acid in 10% hydrochloric acid and water.

Product Safety Labs. 2000. Acute oral toxicity study in rats – limit test. PSL Study No. 8862.

Product Safety Labs. 2000. Acute inhalation toxicity study in rats – limit test. PSL Study No.8864.

Product Safety Labs. 2000. Acute dermal toxicity study in rats – limit test. PSL Study No.8863.

Product Safety Labs. 2000. DOT skin corrosion study in rabbits. PSL Study No.8866.

Product Safety Labs. 2000. Primary eye irritation study in rabbits. PSL Study No.8865.

Elars Bioresearch Laboratories. 1980. 14-Day oral range finding study of PCBTF in rats. Elars Project No. 1603-P.

Raltech Scientific Services. 1979. 14-Day oral range finding study for dose level determination for modified 90-day feeding and reproduction study in rats. Raltech Study No. 79508-A.

Raltech Scientific Services. 1978. p-chlorobenzotrifluoride (PCBTF) and 3,4-dichlrobenzotrifluoride (3,4-DCBTF) 28-day feeding study in rats. Raltech Project No. T-809.

IUCLID
Data Set

CAS# 5216-25-1

Occidental Chemical Corporation

1.0 General Information

1.0.1 Substance Information

A. **CAS No.:** 5216-25-1
B. **Chemical:** Benzene, 1-chloro-4-(trichloromethyl)-
C. **Generic Name:**
D. **EINECS Name:**
E. **Molecular Formula:** $C_7H_4Cl_4$
F. **Molecular Weight:** 229.6

1.02 OECD Information

Company: Occidental Chemical Corporation
Creation date:

Company: Brock Scientific Consulting, LLC on behalf of Occidental Chemical Corp.

Printing Date:
Date of Last Update:

Number of Pages: 22

Chapter (profile): 2, 4, 5
Reliability (profile): without reliability 2

1.03 Details of Chemical Category

1.1 General Substance Information

A. **Type of Substance:** Organic
B. **Physical State:**
C. **Purity:**
D. **Color:**
E. **Odor:**

1.2 Impurities

1.3 Additives

1.4 Synonyms

- 1-Chloro-4-trichloromethylbenzene
- 4-Chlorobenzotrichloride
- PCBTC
- alpha, alpha, alpha-trichloro-4-chlorotoluene

1.5 Quantity

1.6 Use Patterns

1.7 Sources of Exposure

1.8 Additional Information

2.0 Physical-Chemical Data

2.1 Melting Point

2.2 Boiling Point

2.3 Density

2.4 Vapor Pressure

2.5 Partition Coefficient

2.6.1 Water Solubility

2.6.2.1.1 Other Solvents

2.6.2 Surface Tension

2.7 Flash Point

2.8 Auto Flammability

2.9 Flammability

2.10 Explosive Properties

2.11 Oxidizing Properties

2.12 Oxidation/Reduction Potential

2.13 Additional Remarks

Type: Hydrolytic Stability
Method: Unknown
Method: Unknown.
Year: 1981
GLP: No
Test substance: PCBTC (concentration not specified)
Result: The half-life (not defined) of PCBTC in distilled water at 0 °C was 38 min. At 25 °C, the half-life was 1.7 min.
Source: Memo from S. Gelfand, 1981.
Reliability: 4- Not Assignable

3.0 Environmental Fate and Pathways

3.1 Stability

A. **Photodegradation**

B. **Stability in Water**

C. **Stability in Soil**

3.2 Monitoring Data (Environment)

3.3 Transport and Distribution

3.3.1 Transport between Environmental Compartments

3.3.2 Distribution

3.4 Aerobic Degradation

3.5 BOD5, COD or BOD5/COD Ratio

3.6 Bioaccumulation

3.7 Additional Remarks

4.0 Environmental Toxicity

4.1 Acute Toxicity to Fish

Type: Static
Species: Fathead Minnow (*Pimephales promelas*)
Exposure period: 96 hr
LC50: >100 mg/L
Analytical Monitoring: No data
Method: Five fish/replicate exposed in 750 mL to PCBTC at 1, 10 and 100 mg/L for up to 96 hr. There were two replicates/concentration.
Year: 1997
GLP: No
Test substance: PCBTC (purity 99%)
Water Quality Characteristics: Temperature 22.1-23.9 °C; dissolved oxygen 6.6-8.1 mg/L (80-90% saturation at 23 °C); pH 7.66-8.32.
Result: No mortalities occurred. All solutions were clear with no surface film or precipitate. At 100 mg/L small oily droplets were noted in the second replicate although all solutions were clear at 48 hr.
Source: ABC Laboratories, 1997.
Reliability: 2- Reliable with restrictions

4.2 Acute Toxicity to Aquatic Invertebrates

Type: Static
Species: *Daphnia magna*
Exposure period: 48 hr
EC50: 3.6 mg/L
Analytical Monitoring: No data
Method: Five organisms/replicate exposed in 200 mL to PCBTC at 1, 10 and 100 mg/L for 48 hr. There were two replicates/concentration.
Year: 1997
GLP: No
Test substance: PCBTC (purity 99%)
Water Quality Characteristics: Temperature 19.9-22 °C; dissolved oxygen 7.3-8.4 mg/L (84-97% saturation at 23 °C); pH 7.71-8.53.
Result: At 100 mg/L small oily droplets were noted although all solutions were clear at 48 hr. At 100 mg/mL, 100% immobility was observed at 24 hr. Daphnia were immediately affected on addition of 100 mg/mL with all organisms on the bottom of the vessel at 0 hr. The 24-hr EC50 was estimated to be 6.7 mg/mL.
Source: ABC Laboratories, 1997.
Reliability: 2- Reliable with restrictions

4.3 Toxicity to Aquatic Plants

Type: Static
Species: *Selenastrum capricornutum*
Exposure period: 96 hr
EC50: 27 mg/L

Analytical Monitoring: No data
Method: The initial density was 10^4 cells/mL in a 100 mL volume. PCBTC added at 1, 10 and 100 mg/L. There were three replicates/concentration.
Year: 1997
GLP: No
Test substance: PCBTC (purity 99%)
Water Quality Characteristics: Temperature 23.8-24.2 °C; pH 3.6-9.5.
Result: At 100 mg/L small oily droplets were noted although all solutions were clear at 96 hr. The cell counts at 100 mg/mL were less than controls.
Source: ABC Laboratories, 1997.
Reliability: 2- Reliable with restrictions

4.4 Toxicity to Microorganisms

4.5 Chronic Toxicity to Aquatic Organisms

A. Chronic Toxicity to Fish

B. Chronic Toxicity to Aquatic Invertebrates

4.6 Terrestrial Organisms

A. Toxicity to Soil Dwelling Organisms

B. Toxicity to Terrestrial Plants

C. Toxicity to other Non-Mammalian Terrestrial Species

4.6.1 Toxicity to Sediment Dwelling Organisms

4.7 Biological Effects Monitoring

4.8 Biotransformation and Kinetics

4.9 Additional Remarks

5.0 Mammalian Toxicity

5.1 Toxicokinetics, Metabolism and Distribution

Species: Rat
Strain: Sprague Dawley
Sex: Female
Number of Animals: 3

Vehicle: None
Method: Single oral dose administered to 2 fasted rats at 1.5 mg/kg. A third rat was treated with a single oral dose of 102 mg/kg. Animals placed in glass metabolism cages for the collection of urine, feces and expired air. Selected tissues collected after Day 6 urine collection for residual levels of compound.
Year: 1981
GLP: No
Test substance: [U-ring-^{14}C)-p-chlorobenzotrichloride; 98.1% radiochemical purity; specific activity 4 mCi/mmol.
Result: PCBTC was excreted primarily in the urine with 87% eliminated within 6 days. About 9% was eliminated in the feces with <0.002% eliminated in expired air. At the higher dose, 77% and 14% were eliminated in the urine and feces, respectively, by Day 4 after treatment. Only 4% of the administered dose was found in the carcass at Days 4 and 6 following treatment. Little parent compound was eliminated over 6 days (≤1%). Principle metabolite was p-chlorohippuric acid in the urine accounting for about 96% in the first 24 hr. p-Chlorobenzoic acid was observed in the urine with increasing concentrations over 6 days. In the feces, p-chlorobenzoic acid was the primary metabolite although p-chlorohippuric acid was observed at greater levels when the rat was treated with the higher dose. The liver and intestinal contents contained the greatest concentrations of the radiolabel compared to other tissues, accounting for about 0.2% of the dose. Other tissues were generally ≤0.1% of the administered dose.

Radiolabel Balance for Rats Treated with a single Oral Dose of ^{14}C-p-Chlorobenzotrichloride

Tissue	Percent of Administered Dose	
	1.5 mg/kg (n=2)	102 mg/kg (n=1)
Urine	87	77
Feces	9	14
14CO2	≤0.02	ND
Volatile Organics	≤0.02	ND
Total Recovery	100	95

ND=Not Determined

Source: Zoecon Corporation, 1981.
Reliability: 2 - Reliable with restrictions

5.2 Acute Toxicity

A. Acute Oral Toxicity

Type: LD50
Species: Rat
Strain: Sprague Dawley
Sex: Male/Female
Number of Animals: 5/sex
Vehicle: None
Value: 820 mg/kg

Method: Single oral dose administered to fasted rats at doses of 510, 720, 1001 and 1410 mg/kg. Animals observed daily for 14 days for clinical signs of toxicity and mortality. Gross necropsy of the thoracic and abdominal cavities conducted at day 14.
Year: 1980
GLP: Yes
Test substance: PCBTC (97.4% pure)
Result: Mortalities occurred at 720 mg/kg and greater. Clinical signs of toxicity were noted and included decreased motor activity, tremors diarrhea, piloerection and chromodacryorrhea. All animals gained weight during the 14-day observation time. No gross abnormalities were observed. Gastrointestinal irritation observed in most rats in the 1001 and 1410 mg/kg groups. No gross necropsy findings were noted in rats treated with the lower doses.
Source: Springborn Institute for Bioresearch, 1980.
Reliability: 2 - Reliable with restrictions

B. Acute Inhalation Toxicity

C. Acute Dermal Toxicity

Type: LD50
Species: Rabbit
Strain: New Zealand White
Sex: Male/Female
Number of Animals: 2/sex
Vehicle: None
Value: >2000 mg/kg
Method: Single topical dose at 2000 mg/kg under an occlusive patch was applied to intact and abraded skin of 2 rabbits (1/sex) each for 24 hr. Animals observed daily for 14 days for clinical signs of toxicity and mortality. Gross necropsy of the thoracic and abdominal cavities conducted at day 14.
Year: 1980
GLP: Yes
Test substance: PCBTC (97.4% pure)
Result: No mortalities were observed. No clinical signs of toxicity were noted. Slight to mild erythema and edema (Draize scores of 1 and 2) were observed throughout the study. Fissuring of the skin or desquamation was noted in some rabbits. No gross abnormalities were observed.
Source: Springborn Institute for Bioresearch, 1980.
Reliability: 2 - Reliable with restrictions

D. Acute Toxicity, Other Routes

5.3 Corrosiveness and Irritation

A. Skin Irritation

Species: Rabbit
Strain: New Zealand White
Concentration: 100%
Dose: 0.5 mL
Exposure Time: 24 hr
Number of Animals: 6 rabbits; sex not specified
Classification: Irritant
Method: The test substance applied to the intact or abraded skin of rabbits. The sites were occluded for 24 hr. The patch was removed and any residual substance removed with water. All sites were evaluated for irritation/corrosion at 24 and 72 hr following patch removal. Irritation scored by the method of Draize.
Year: 1980
GLP: Yes
Test substance: PCBTC (97.4% pure)
Result: Very slight (Draize score of 1) erythema and very slight to slight edema (Draize scores of 1 and 2, respectively) were observed in all test sites at 24 and 72 hr. The primary irritation value was 1.58 (maximum score of 8).

Irritation Scores - Intact Skin

Animal Number	Time after Patch Removal (hr)	
	24 hr	72 hr
71480	1/0	0/0
71580	1/1	1/0
71880	1/1	1/0
72080	1/1	1/1
72180	1/1	0/1
72380	1/1	0/0

* Draize scores presented as erythema/edema

Irritation Scores - Abraded Skin

Animal Number	Time after Patch Removal (hr)	
	24 hr	72 hr
71480	1/0	1/0
71580	1/1	1/0
71880	1/1	1/1
72080	½	1/1
72180	1/1	0/1
72380	1/2	1/1

* Draize scores presented as erythema/edema

Source: Springborn Institute for Bioresearch, 1980.
Reliability: 2 - Reliable with restrictions

Species: Rabbit
Strain: New Zealand White
Concentration: 100%
Dose: 0.5 mL
Exposure Time: 4 hr
Number of Animals: 6 rabbits; 3/sex
Classification: Irritant
Method: The test substance applied to the intact or abraded skin of rabbits. The sites were semi-occluded for 4 hr. The patch was removed and any residual substance removed with water. All sites were evaluated for irritation/corrosion at 0, 5, 24, 48 and 72 hr and 7, 14 and 21 days following patch removal. Irritation scored by the method of Draize.
Year: 2000
GLP: Yes
Test substance: PCBTC (99% pure)
Result: No irritation was observed through 24 hr following patch removal. Slight to well-defined erythema (Draize scores 1 and 2, respectively) were observed at 48 hr. No edema was observed throughout the study except slight edema (Draize score 2) was noted in 3 rabbits only at day 7. Erythema was noted in all rabbits through day 14 with moderate erythema observed in one rabbit on day 7. All irritation resolved by day 21. There was no difference in the irritation response observed in the intact and abraded skin sites. The primary irritation value was 2.2 for intact skin and 2.0 for abraded skin (maximum score of 8).

Irritation Scores – Intact Skin

Animal Number	Time After Patch Removal							
	Hours					Days		
	0	5	24	48	72	7	14	21
1171	0/0	0/0	0/0	1/0	1/0	2/2	1/0	0/0
1172	0/0	0/0	0/0	2/0	1/0	2/0	2/0	0/0
1173	0/0	0/0	0/0	2/0	1/0	1/0	1/0	0/0
1174	0/0	0/0	0/0	1/0	1/0	2/2	1/0	0/0
1175	0/0	0/0	0/0	2/0	1/0	3/2	1/0	0/0
1176	0/0	0/0	0/0	1/0	1/0	1/0	1/0	0/0

* Draize scores presented as erythema/edema

Irritation Scores – Abraded Skin

Animal Number	Time After Patch Removal							
	Hours					Days		
	0	5	24	48	72	7	14	21
1171	0/0	0/0	0/0	1/0	1/0	2/2	1/0	0/0
1172	0/0	0/0	0/0	2/0	2/0	2/0	2/0	0/0
1173	0/0	0/0	0/0	2/0	1/0	2/0	0/0	0/0
1174	0/0	0/0	0/0	1/0	1/0	1/0	1/0	0/0
1175	0/0	0/0	0/0	2/0	1/0	3/2	1/0	0/0
1176	0/0	0/0	0/0	1/0	1/0	1/0	1/0	0/0

* Draize scores presented as erythema/edema

Source: MPI Research 2000.
Reliability: 1 - Reliable without restrictions

B. Eye Irritation

Species: Rabbit
Strain: New Zealand White
Concentration: 100%
Dose: 0.1 mL
Exposure Time: After instillation, the eyes were held closed for about 1 sec.
Number of Animals: 9 rabbits; sex not specified
Classification: Irritant
Method: The test substance was instilled into the conjunctival sac of the right eye of 6 rabbit; the left eye served as the control. After instillation, the eyes of three additional rabbits were washed with water for about 5 sec. Ocular irritation was evaluated at 1, 2, 3, 7 and 14 days following instillation. The ocular irritation of one rabbit was scored on day 21. Irritation scored by the method of Draize. The maximum score was calculated as the sum of all scores for the cornea, iris and conjunctivae. The maximum score is 110. The average maximum score was calculated by dividing the total score by the number of animals evaluated.
Year: 1980
GLP: Yes
Test substance: PCBTC (97.4% pure)
Result: No corneal opacity or iritis was observed during the study. Conjunctivitis was noted in all treated eyes. By day 21, all irritation had resolved. The maximum average score was 10.3 for the unwashed eye and 10.7 for the washed eye.

Ocular Irritation Scores – Unwashed Eye

Rabbit Number	Scoring Time (Day)	Corneal Opacity	Iritis	Conjunctiva		
				Redness	Chemosis	Discharge
719-80	1	0	0	2	1	0
	2	0	0	1	1	0
	3	0	0	2	2	0
	7	0	0	1	2	0
	14	0	0	0	0	0
721-80	1	0	0	2	3	1
	2	0	0	2	2	1
	3	0	0	3	3	2
	7	0	0	2	3	1
	14	0	0	0	0	0
722-80	1	0	0	2	2	1
	2	0	0	2	2	0
	3	0	0	2	2	0
	7	0	0	2	2	0
	14	0	0	1	0	0
	21	0	0	0	0	0
723-80	1	0	0	2	2	0
	2	0	0	2	2	2
	3	0	0	1	2	1
	7	0	0	2	3	0
	14	0	0	0	0	0
725-80	1	0	0	2	1	0
	2	0	0	2	2	1
	3	0	0	2	2	1
	7	0	0	2	3	0
	14	0	0	0	0	0
726-80	1	0	0	2	1	0
	2	0	0	2	2	1
	3	0	0	2	2	2
	7	0	0	2	3	0
	14	0	0	0	0	0

Ocular Irritation Scores – Washed Eye

Rabbit Number	Scoring Time (Day)	Corneal Opacity	Iritis	Conjunctiva		
				Redness	Chemosis	Discharge
727-80	1	0	0	2	2	1
	2	0	0	2	2	0
	3	0	0	2	2	0
	7	0	0	2	3	0
	14	0	0	0	0	0
728-80	1	0	0	2	3	1
	2	0	0	2	2	2
	3	0	0	2	2	0
	7	0	0	2	3	0
	14	0	0	0	0	0
730-80	1	0	0	2	2	1
	2	0	0	2	2	1
	3	0	0	1	2	0
	7	0	0	2	2	0
	14	0	0	0	0	0

Source: Springborn Institute for Bioresearch, 1980.
Reliability: 2 - Reliable with restrictions

Species: Rabbit
Strain: New Zealand White
Concentration: 100%
Dose: 0.1 mL
Exposure Time: After instillation, the eyes were held closed for about 1 sec.
Number of Animals: 6 rabbits; 3/sex
Classification: Irritant
Method: The test substance was instilled into the conjunctival sac of the right eye of 6 rabbit; the left eye served as the control. After instillation, the eyes of three rabbits were washed with water for about 5 sec. Ocular irritation was evaluated at 1, 24, 48 and 72 hr and at 4, 7, 14 and 21 days following instillation. Fluroescein examinations were conducted at 24 and 72 hr and at 7, 14 and 21 days. The ocular irritation of one rabbit was scored on day 21. Irritation scored by the method of Draize. The maximum score was calculated as the sum of all scores for the cornea, iris and conjunctivae. The maximum score is 110. The average maximum score was calculated by dividing the total score by the number of animals evaluated.
Year: 1980
GLP: Yes
Test substance: PCBTC (99% pure)
Result: No iritis was observed in the washed or unwashed eye, and no corneal opacity was noted in washed eye during the study. Conjunctivitis was noted in the washed eye of all treated eyes. By day 21, all irritation had resolved. In the unwashed eye, diffuse corneal opacity was noted at 72 hr and 4 days post-instillation. Diffuse redness, discharge and moderate swelling with partial eversion of the lids of the conjunctivae were noted in the treated rabbits. Fluroescein examination of the washed eyes revealed 0% staining at

all intervals except that 1 animal exhibited 5% staining at 72 hr. In the unwashed eye, no fluroescein staining was noted except that 10% staining in one rabbit and 5% staining in another animal was observed at 72 hr. The maximum average score was 13 for the unwashed eye and 18 for the washed eye at 1 hr and 4 days, respectively.

Ocular Irritation Scores – Washed Eye

Rabbit Number	Scoring Time	Corneal Opacity	Iritis	Conjunctiva		
				Redness	Chemosis	Discharge
1165	1 hr	0	0	3	4	3
	24 hr	0	0	1	1	0
	48 hr	0	0	1	1	0
	72 hr	0	0	1	1	2
	4 day	0	0	2	2	2
	7 day	0	0	3	2	0
	14 day	0	0	0	0	0
	21 day	0	0	0	0	0
1166	1 hr	0	0	3	3	3
	24 hr	0	0	2	1	0
	48 hr	0	0	2	1	2
	72 hr	0	0	3	2	3
	4 day	0	0	3	2	2
	7 day	0	0	3	2	0
	14 day	0	0	1	0	0
	21 day	0	0	0	0	0
1167	1 hr	0	0	3	3	2
	24 hr	0	0	2	2	0
	48 hr	0	0	2	1	2
	72 hr	0	0	2	2	2
	4 day	0	0	3	2	2
	7 day	0	0	3	2	1
	14 day	0	0	1	0	0
	21 day	0	0	0	0	0

Ocular Irritation Scores – Unwashed Eye

1168	1 hr	0	0	2	2	1
	24 hr	0	0	2	2	1
	48 hr	0	0	3	2	2
	72 hr	1	0	3	2	2
	4 day	1	0	3	2	2
	7 day	0	0	3	2	0
	14 day	0	0	0	0	0
1169	1 hr	0	0	3	2	2
	24 hr	0	0	2	1	0
	48 hr	0	0	1	1	0
	72 hr	0	0	2	1	0
	4 day	0	0	2	1	1
	7 day	0	0	2	1	0
	14 day	0	0	0	0	0
	21 day	0	0	0	0	0
1170	1 hr	0	0	2	2	1
	24 hr	0	0	2	2	1
	48 hr	0	0	2	2	2
	72 hr	0	0	2	2	2
	4 day	0	0	2	2	2
	7 day	0	0	2	2	0
	14 day	0	0	1	0	0
	21 day	0	0	0	0	0

Source: MPI Research, 2000.
Reliability: 1 - Reliable without restrictions

5.4 Sensitization

Species: Guinea pig
Strain: Hartley
Induction Concentration: 5% in acetone
Challenge Concentration: 0.1% in acetone
Dose: 0.4 mL
Exposure Time: 6 hr
Number of Animals: 10/sex
Classification: Weak sensitizer
Method (Buehler): For induction, the test substance was applied to the intact skin under an occlusive patch for 6 hr. This procedure was repeated once a week for 2 additional weeks. Two weeks after the last induction application, the challenge concentration was applied to a naïve site under an occlusive patch for 6 hr. The sites were evaluated for irritation at 24 and 48 hr following patch removal. The challenge concentration was based on a preliminary irritation study in naïve guinea pigs. Irritation scores were based on the method of Draize.

Year: 1981
GLP: Yes
Test substance: PCBTC
Result: No irritation was observed in control animals at challenge. In the PCBTC animals,

slight erythema was observed in most animals are 24 and 48 hr following challenge. Two animals died prior to challenge, but the deaths were not related to the compound.

Incidence of Irritation in Guinea Pits Challenged with 0.1% PCBTC

Sex	24 hr	48 hr
Male	8/9*	7/9
Female	6/8	5/8

* Incidence of guinea pigs with irritation (±) over the total number of animals challenged with PCBTC

Source: MPI Research, 2000.
Reliability: 2 - Reliable with restrictions

5.5 Repeated Dose Toxicity

5.6 Genetic Toxicity 'in Vitro'

A. Gene Mutation

B. Chromosomal Aberration

5.7 Genetic Toxicity 'in Vivo'

5.8 Carcinogenicity

5.9 Toxicity to Reproduction

A. Fertility

B. Developmental Toxicity/Teratogenicity

Species: Rat
Strain: Not specified
Number: 8 females/group
Route of administration: Inhalation
Exposure period: 6-19 Days of Gestation (GD)
Frequency of treatment: Daily
Concentrations: 15, 30, 60 µg/L
Control Group: Air
NOAEL: 15 µg/L
Method: Rats were exposed by inhalation for 6 hr/day on GD 6-19. On GD 20, the animals were sacrificed and the fetuses examined for external malformations, corpora lutea, fetal death, sex ratio, pre- and post-implantation loss and body weights. In parental rats, pregnancy rate, body weights, food consumption and clinical signs of toxicity were recorded.
Year: 1984

GLP: No data
Test substance: PCBTC
Result: In parental animals at 60 µg/L, a significant decrease in body weights and food and water consumption were observed during the exposure phase. Two rats in the high-dose group died prior to sacrifice on Day 20 and the remaining animals had premature births. Clinical signs of toxicity were evident during the exposure phase and included hunched posture, aggressiveness, tremors and labored respiration. At 30 µg/L, no mortalities or clinical signs of toxicity were observed although decreases in body weights and food consumption were noted. No effects on parental animals were observed at 15 µg/L. At 30 µg/L , fetal body weights were lower than controls. No effects on other litter data values or external malformations were evident. No fetuses survived at 60 µg/L.

Mean Litter Data from Rats Exposed by Inhalation to PCBTC

PCBTC Exposure Concentration (µg/L)	Pregnancy Rate	Viable Fetuses	Total Resorptions	Premature Births	Implantations	Corpora Lutea	Pre-Implantation Loss (%)	Fetal Loss (%)	Litter Weight (g)	Mean Fetal Weight (g)
Control	100	11.5	0.6	0	12.1	12.8	5.2	4.5	39.65	3.48
15	87.5	11.3	0.6	0	11.9	12.3	3.1	4.2	39.09	3.48
30	100	11.0	0.6	0	11.6	12.9	7.9	5.5	34.35	3.12
60	100	0	0.2	10	10.2	11.5	11.2	100	ND	ND

ND – Not Determined as all fetuses were dead

Source: Huntingdon Research Centre, 1984.
Reliability: 1- Reliable without restrictions

Species: Rat
Strain: Crl:COBS CD (SD) BR
Number: 25 females/group
Route of administration: Inhalation
Exposure period: 6-19 Days of Gestation (GD)
Frequency of treatment: Daily
Concentrations: 4, 10, 25 µg/L
Control Group: Air
NOAEL: 10 µg/L
Method: Rats were exposed by inhalation for 6 hr/day on GD 6-19. On GD 20, the animals were sacrificed and the fetuses examined for visceral and skeletal malformations, corpora lutea, fetal death, sex ratio, pre- and post-implantation loss and body weights. In parental rats, pregnancy rate, body weights, food consumption and clinical signs of toxicity were recorded. Exposure concentrations based on preliminary study described above.
Year: 1984
GLP: Yes
Test substance: PCBTC
Result: In parental animals, body weights and food consumption were reduced at the high concentration. No compound-related effects were observed on clinical signs of toxicity or on pregnancy rate. No compound-related macroscopic findings were evident. Litter and mean fetal weights were lower at 25 µg/L compared to controls. Also, a slight increase in the incidences of cervical rib and sternebrae skeletal variations was noted at the high concentration. This increase was considered by the author to be related to the lower fetal body weights. No other PCBTC-related effects were observed.

Litter and Mean Fetal Body Weights

PCBTC Exposure Concentration (µg/L)	Number of Live Young	Letter Weight (g)	Mean Fetal Weights (g)
Control	11.5	37.94	3.30
4	12.1	39.43	3.27
10	12.0	38.44	3.21
25	11.2	34.24	3.05*

* Significantly different from controls ($p<0.01$) by Kruskal-Wallis test

Mean Incidence of Fetal Malformations and Anomalies

PCBTC Exposure Concentration (µg/L)	Number of Litters	Number of Fetuses									
		Malformations			Anomalies						
					Visceral			Skeletal			
		Examined	Total	Mean %	Examined	Total	Mean %	Examined	Total	Mean %	Number Fetuses with Cervical Rib
Control	19	218	3	1.4	108	0	0	107	15	15	0
4	19	229	3	1.3	115	1	0.8	111	30	28	0
10	21	253	1	0.4	129	6	5.7	123	29	23.2	0.8
25	22	246	1	0.9	124	7	9.2	121	29	22.6	7.3
Historical Control Values (Range)							4.2-14.3			3.2-30.6	

Mean Fetal Incidence of Skeletal Variations

PCBTC Exposure Concentration (µg/L)	Fetuses Examined	Fetuses with Finding					
		Normal Sternebrae		Unossified Sternebrae		Total Variant Sternebrae	
		Number	Percent	Number	Percent	Number	Percent
Control	107	29	27.1	55	51.8	78	72.9
4	111	13	12.2	74	67	98	87.8
10	123	17	13.7	80	65.6	106	86.3
25	121	4	3.1*	105	84.6*	117	96.9*

* Significantly different from controls ($p<0.01$) by Kruskal-Wallis test

Source: Huntingdon Research Centre, 1984.
Reliability: 1- Reliable without restrictions

5.10 Other Relevant Information

A. Neurotoxicity

B. Other

5.11 Experience with Human Exposure

6.0 References:

ABC Laboratories. 1997. Acute toxicity of PCBTC to fathead minnows (*Pimephales promelas), Daphnia magna* and *Selenastrum capricornutum* (freshwater algae). ABC Study No. 44103, 44104, 44105.

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Springborn Institute for Bioresearch, Inc. 1980. Dermal toxicity (LD50) in rabbits of parachlorotoluene, dichlorotoluene and parachlorobenzotrichloride. SIB Study No. 3090.2.

Springborn Institute for Bioresearch, Inc. 1980. Eye irritation study of parachlorotoluene, dichlorotoluene and parachlorobenzotrichloride. SIB Study No. 3090.3.

Springborn Institute for Bioresearch, Inc. 1980. Rabbit primary skin irritation of parachlorotoluene, dichlorotoluene and parachlorobenzotrichloride. SIB Study No. 3090.4.

Springborn Institute for Bioresearch, Inc. 1981. Delayed contact hypersensitivity of parachlorobenzotrichloride and dichlorotoluene. SIB Study No. 3090.5.

Zoecon Corp. 1981. Metabolism of p-chlorobenzotrichloride in rats. Zoecon Report No. 7271-28A-10-13-81.

IUCLID
Data Set

CAS# 25168-05-2

Occidental Chemical Corporation

1.0 General Information

1.0.1 Substance Information

A. **CAS No.:** 25168-05-2
B. **Chemical:** Benzene, chloromethyl-
C. **Generic Name:** Chlorotoluene
D. **EINECS Name:**
E. **Molecular Formula:** C_7H_7Cl
F. **Molecular Weight:** 126.5

1.02 OECD Information

Company: Occidental Chemical Corporation
Creation date:

Company: Brock Scientific Consulting, LLC on behalf of Occidental Chemical Corp.

Printing Date:
Date of Last Update:

Number of Pages: 8

Chapter (profile): 2, 3, 5
Reliability (profile): Without reliability 2, 3, 5

1.03 Details of Chemical Category

1.1 General Substance Information

A. **Type of Substance:** Organic
B. **Physical State:**
C. **Purity:**
D. **Color:**
E. **Odor:**

1.2 Impurities

1.3 Additives

1.4 Synonyms

1.5 Quantity

1.6 Use Patterns

1.7 Sources of Exposure

1.8 Additional Information

2.0 Physical-Chemical Data

2.1 Melting Point

2.2 Boiling Point

2.3 Density

2.4 Vapor Pressure

2.5 Partition Coefficient

Value: 3.1562 for o-chlorotoluene; 3.147 for p-chlorotoluene
Qualitative: Calculation
Method: Calculated based on empirical equation of Chiou (1977).

log Kow = 5.0 – 0.67log WS where the logWS is the water solubility in µmol/L

Year: 1981
GLP: No
Result: T
Source: Gelfand, 1981.
Reliability: 4 – Not Assignable

2.6.1 Water Solubility

2.6.2.1.1 Other Solvents

2.6.2 Surface Tension

2.7 Flash Point

2.8 Auto Flammability

2.9 Flammability

2.10 Explosive Properties

2.11 Oxidizing Properties

2.12 Oxidation/Reduction Potential

2.13 Additional Remarks

3.0 Environmental Fate and Pathways

3.1 Stability

A. Photodegradation

B. Stability in Water

C. Stability in Soil

3.2 Monitoring Data (Environment)

3.3 Transport and Distribution

3.3.1 Transport between Environmental Compartments

3.3.2 Distribution

Type: Soil Absorption Coefficient
Method: Soil absorption coefficient (Koc) was calculated for o- and p-chlorotoluene based on water solubility values. The values were calculated according to the equation:

log Koc = 0.44 – 0.54log WS where the logWS is the mole fraction water solubility

Year: 1981
GLP: No
Test substance: No data
Result: The Koc for o-chlorotoluene was 884 and for p-chlorotoluene 865.
Source: Gelfand, 1981
Reliability: 4 – Not Assignable

3.4 Aerobic Degradation

3.5 BOD5, COD or BOD5/COD Ratio

3.6 Bioconcentration

Type: Soil Absorption Coefficient
Method: Bioconcentration factor (BCF) was calculated for o- and p-chlorotoluene based on water solubility values. The values were calculated according to the equation:

log Koc = 3.995 – 03891log WS where the logWS is the ppm water solubility

Year: 1981
GLP: No
Test substance: No data
Result: The BCF for o-chlorotoluene was 128 and for p-chlorotoluene 126.
Source: Gelfand, 1981
Reliability: 4 – Not Assignable

3.7 Additional Remarks

4.0 Environmental Toxicity

4.1 Acute Toxicity to Fish

4.2 Acute Toxicity to Aquatic Invertebrates

4.3 Toxicity to Aquatic Plants

4.4 Toxicity to Microorganisms

4.5 Chronic Toxicity to Aquatic Organisms

A. Chronic Toxicity to Fish

B. Chronic Toxicity to Aquatic Invertebrates

4.6 Terrestrial Organisms

A. Toxicity to Soil Dwelling Organisms

B. Toxicity to Terrestrial Plants

C. Toxicity to other Non-Mammalian Terrestrial Species

4.6.1 Toxicity to Sediment Dwelling Organisms

4.7 Biological Effects Monitoring

4.8 Biotransformation and Kinetics

4.9 Additional Remarks

5.0 Mammalian Toxicity

5.1 Toxicokinetics, Metabolism and Distribution

5.2 Acute Toxicity

A. Acute Oral Toxicity

B. Acute Inhalation Toxicity

C. Acute Dermal Toxicity

D. Acute Toxicity, Other Routes

5.3 Corrosiveness and Irritation

A. Skin Irritation

B. Eye Irritation

5.4 Sensitization

5.5 Repeated Dose Toxicity

Species: Rats
Strain: Charles River
Sex: Male and female
Route of administration: Gavage
Exposure period: 14 Days
Frequency of treatment: Daily
Observation period: 90 Days
Doses: 100, 300 and 1000 mg/kg
Control Group: Corn oil (0.2 mL/100 g body weight)
NOAEL: 100 mg/kg based on body weight reduction
Method: Rats (15/sex/group) were treated daily by gavage at a dose volume of 0.2 mL/100 g body weight. The animals were observed daily for clinical signs of toxicity and moribundity and mortality. Body weights were recorded weekly, and food consumption was determined weekly for 5 rats/sex/group. Blood was collected from 10/sex/group for clinical pathology on days 40 and 90. Urine was collected from 10 rat/sex in the 100 and

300 mg/kg groups. Organ weights collected for the brain, sex organs, heart, kidneys, liver and spleen. The animals were subjected to a gross necropsy, and the spleen, liver and kidneys weighed.

Year: 1977

GLP: No

Test substance: Monochlorotoluene (51% o-chlorotoluene, 48% p-chlorotoluene)

Result: Slight decreases in body weights and body weight gains of rats in the 300 and 1000 mg/kg groups. Four rats were died during the study but deaths were not compound-related. No effects were observed on clinical signs of toxicity or on clinical pathology measures or organ weights. No gross microscopic pathology findings were observed.

Source: Industrial Bio-Test Laboratories, 1977.

Reliability: 3- Not Reliable

5.6 Genetic Toxicity 'in Vitro'

A. Gene Mutation

B. Chromosomal Aberration

5.7 Genetic Toxicity 'in Vivo'

5.8 Carcinogenicity

5.9 Toxicity to Reproduction

A. Fertility

B. Developmental Toxicity/Teratogenicity

5.10 Other Relevant Information

A. Neurotoxicity

B. Other

5.11 Experience with Human Exposure

6.0 References:

Chiou, C.T., et al., Environ, Sci. Tech. 11: 477.

Gelfand, S. 1981. Monochlorotoluenes: Water solubilities and related properties (octanol/water partition coefficient, bioconcentration factor and soil absorption). Hooker Chemical Co., Report 48460

Industrial Bio-Test Laboratories, Inc. 1977. 90-Day Subacute oral toxicity study with monochlorotoluene isomers in albino rats. Study No. 8532-08283.